Oxygen *K* Emission spectra of Sr_2CuO_3

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INTRODUCTION

The fundamental physical properties of low-dimensional and correlated systems have attracted a lot of interest in recent years [1-3]. Ladder-type copper-oxide materials form an interesting class of compounds that combine one-dimensionalies (1D) with electronic correlations. Experimentally, Sr_2CuO_3 is found to be the best realizations of the quasi-1D spin-1/2 antiferromagnetic Heisenberg model.

Figure 1 shows the structure of the Cu-O chains in Sr_2CuO_3. These chains are comprised of one copper and two inequivalent oxygen atoms denoted as O(1) and O(2). Chains of oxygen corner sharing CuO_4 plaquettes run along the *b* direction and the parallel Cu-O chains shift along the *a* direction.

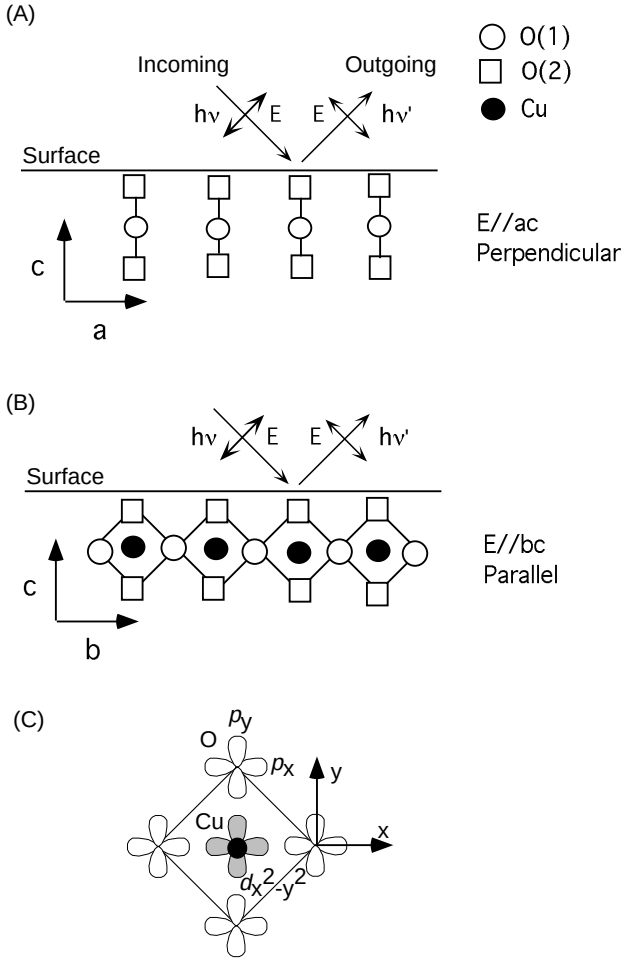

Figure 1. Structure of Cu-O chains in Sr_2CuO_3. (A) *E* //*ac* arrangement. (Perpendicular). (B)*E* //*bc* arrangements. (Parallel). (C) Configuration of the O $2p_x$, p_y and Cu $3d_{x^2-y^2}$ orbitals.

Soft x-ray emission (SXE) spectroscopy with tunable excitation allows one to study occupied electronic structure of a specific atomic site in a compound [4]. In this work, we have recorded oxygen $K\alpha$ emission spectra of Sr_2CuO_3 in two arrangements (see Fig. 1) with various incident angles.

EXPERIMENTAL

The oxygen $K\alpha$ spectra of Sr_2CuO_3 single crystal were recorded using a high-resolution grazing incidence x-ray fluorescence spectrometer [5] at beamline 7.0. During the O $K\alpha$ SXE measurements, the resolution of the beamline was 0.5 eV and the resolution of the fluorescence spectrometer was set to 0.4 eV.

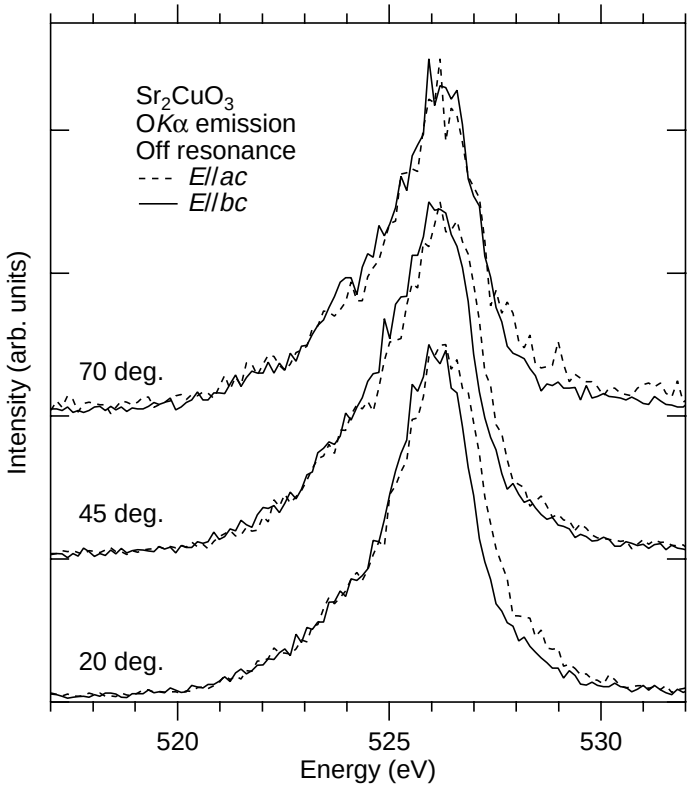

Figure 2. The off resonance O $K\alpha$ soft-x-ray-emission spectra of Sr_2CuO_3 with various incident x-ray angles.

Two geometry of Sr_2CuO_3 were measured with various incident angle. In the arrangements, one is in the *E*//*ac* arrangement in which the incident photon polarization *E* is in the *ac* plane and perpendicular to the chain (Fig. 1, (A)) and another is in the *E*//*bc* arrangement in which *E* is in the *ab* plane and has a component parallel to the chain (Fig. 1, (B)). The incidence angle of the photon beam was about 20, 45, and 70 degrees to the sample surface, here incoming angle + outgoing angle = 90 deg.

The experiments were performed at room temperature with a base pressure of 4×10^{-8} Torr in the experimental chamber. The clean surface was prepared by cleaving just before introduction into the vacuum chamber.

RESULTS

Figure 2 show the O $K\alpha$ SXE spectra of Sr_2CuO_3 in two arrangements with various incident x-ray angles. The energy of excitation was 9 eV above the O 1*s* threshold, with this excitation energy only O 2*p* -> O 1*s* transitions are possible and the spectra are regarded as excited off resonance. The intensities of the spectra are normalized to the peak maximum. Dashed and solid curves show the spectra in *E*//*ac* and *E*//*bc* arrangements, respectively.

The significant differences are observed in the O $K\alpha$ spectra recorded with incident angle of 20 deg. (outgoing angle of 70 deg.), at the high-energy side (526-529 eV) the *E*//*ac* spectra have higher intensity than that of the *E*//*bc* spectra. At off resonance condition with low incident angle (20 degrees), O $2p_z$ and $2p_x$ orbitals contribute mainly for the *E*//*ac* and the *E*//*cb* arrangements, respectively. Therefore, the O $K\alpha$ intensity around 526-528 eV is attributed to O $2p_z$ orbital which hybridized with Cu $3d_{yz}$ and d_{zx} orbitals.

At higher incident angle (70 degrees), no intensity difference around 526-528 eV between two arrangements is detected which is consistent with that the O $2p_y$ orbital can contribute for the both *E*//*ac* and the *E*//*bc* arrangements. The difference around 529 eV may be attributed to the Zhang-Rice singlet state which is the hybridized orbital O $2p_y$ with Cu $3d_{x^2-y^2}$.

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